Book Review

Encyclopedia of Computational Chemistry. *P. v. R. Schleyer, editor-in-chief, John Wiley & Sons, Chichester, UK, 1998, 3,500 pp. $3,150. ISBN: 0-471-96588-X.*

Computational chemistry has existed in one form or another for over 40 years. Although this is an interdisciplinary science, it can now be considered in its own right as a stand-alone discipline for several reasons, one of which is now having its own encyclopedia. The *Encyclopedia of Computational Chemistry* is a multieditor effort containing (1) overviews, (2) definition entries, and (3) descriptions of software entries covering various topics in computational chemistry.

Paul Schleyer is the Editor-in-Chief of ECC who assembled the editorial team of N. L. Allinger, T. Clark, J. Gasteiger, P. A. Kollman, and H. F. Schaefer III to assist him. Each editor was responsible for about one-sixth of the chapters as well as writing individual synopses that provide background information, make the connections between various chapters, justify the content of the encyclopedia, afford historical accounts, and to somewhat espouse their philosophies on the topic of computational chemistry. The expertise of these editors covers a good portion of the computational chemistry landscape as we know it today, but they have also asked for additional input from others in the scientific community about topics and authors to be included in this encyclopedia. The final product reflects the care and deep commitment made by the editorial team in this regard; this is a very complete, nonbiased and "community-driven" collaborative effort to identify and explain, in simple terms, the many aspects of computational chemistry that would "... instruct the general user and to facilitate investigations" revealed by the editor-in-chief to be one of the main purposes of this encyclopedia. The editors have nicely correlated the entry of contributions from about 450 contributing authors who are among the prominent leaders in the field of computational chemistry. At the outset I need to tell you that the editors have succeeded in many ways in this bold endeavor, and I highly recommend this encyclopedia.

The encyclopedia looks and feels like an encyclopedia; it consists of five large (8-1/2″ by 11″) books containing over 3400 pages, weighing about 30 pounds total, printed on heavy-duty paper that will ensure its durability for the many students for whom this seems directed. It contains topics in alphabetical order with substantial crossreferencing, an adequate index, and a section at the end of the encyclopedia of promotional features from software developers and vendors who were invited to contribute such information. The books are aesthetic to the hand as well as to the eye; the easy-to-read print, good use of headings and subheadings, and the judicious selection of color all contribute to the luxurious "feel" of the book

More important, though, is its content. In particular, one wants to know if the material presented is technically correct, and also if the book is useful. To assess this I decided to carry out three "experiments." First, I would read some of the entries covering topics that I am knowledgeable about to see if the author was able to summarize in a useful, concise, and correct manner the topic at hand. Second, I would select several entries I knew nothing about to see if I was capable of learning those topics without being overwhelmed by jargon, technical details beyond the expected encyclopedic content, and if suitable references were provided so that I could further pursue the topic if I wanted to. Third, I would ask some colleagues and students to look up a topic of their choice and see what their reactions were to that entry. Here is what I discovered.

My first reading was on "molecular mechanics." This entry was a bit problematic; rather than being a self-contained description of the method, it defined what molecular mechanics is and then indicated where else in the encyclopedia one should go to learn about it. Confusing the issue is that an entry about molecular mechanics treatments of conjugated systems immediately follows the entry on molecular mechanics itself. Hence, all of what one

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needs to know about this topic is in the encyclopedia but not quite where one would expect to find it.

The next topics I looked at were "conformational analysis" and "Cambridge Structural Database." The entry on conformational analysis consists of three parts: conformational analysis:1 by Kolossváry and Guida; conformational analysis:2 by Vajda, and conformational analysis:3 by Eliel. I give all these entries a strong "thumbs up." There exists some redundancy between these chapters, but not much; each chapter provides a different perspective of this amazingly complex topic, and the integration of the three chapters into the encyclopedia is beautifully orchestrated. All three entries are well written, concise, technically superb, and containing many leading references. The entry on the Cambridge Structural Database by Allen and Hoy was likewise stellar. It provided a history of CSD, what the CSD contains, what the software can do, and then provides some research applications, recent developments, and what developments will appear in the near future. Like most of the other entries I scanned in this encyclopedia, the material is technically sound, the writing style is concise but not terse, the text is essentially error-free and the references contain seminal works, key papers, and reviews, and good leading references for follow-up.

My second experiment was to read an entry or two about something I did not know about to see how easily I could grasp the fundamental concepts of that topic. The first entry I read was on Comparative Molecular Field Analysis (CoMFA), written by Kubinyi. Following an introduction that puts its need into perspective, the methodology and application is given, followed by major sections covering: series design and test set selection; pharmacophore hypotheses and alignment; box, grid size, and 3D field calculations; derivation and validation of 3D QSAR models; and applications in drug design. Also enumerated for the novice are additional notes and some practical problems in appropriately labeled subsections. Not only did I become aware of what I can do with the method, I was taught about pitfalls to avoid, given pointers and hints about how to be successful, and provided with ample citations to further pursue this topic. Overall, this was a stellar summary, and, like several other topics I then read about, I was able to quickly get the gist of what the computational method was used for and how it worked.

The third experiment I conducted was to ask some colleagues to look up a topic of interest and tell me what they felt about it. The first topic reviewed by one of my colleagues was "polarizability." A skimpy, completely unsatisfactory definition and explanation was provided. The next topics evaluated were "autodock" and "logP." The former was cited but not described, and the latter was mentioned in an entry on Environmental Chemistry: QSAR. Yet another topic looked for was "lipophilicity." It was missing from the index as well as the main body of the text, but, one could find out more about it by reading the entry on "octanol/water partition coefficients" if one were to have the savvy to do look it up there. The next person I asked was a student who is in the midst of writing a thesis on nonlinear dynamics. She looked up "graph theory," and because she will soon move as a faculty member to a liberal arts college she also looked up "electronegativity." In both cases she was very impressed with the completeness of the descriptions as well as the utility of the encyclopedia for general student use. Both entries were readable, beginning with very basic ideas, guiding her throughout the intricacies of these topics. Both entries were also well illustrated, having high quality pictures that made clear the conceptual ideas being described in the text. Several other "thumbs up" were acquired from other reviewers from local industry as well as from students.

My "experiments" revealed to me that this encyclopedia is very useful; the encyclopedia was found by me, my colleagues, and students to be of great value to our research and educational missions at a university, and it can be of great use in an industrial setting as well. The physical and aesthetic attributes of the book itself, its content, and usefulness, especially for the novice, are all excellent despite some weak entries and inconsistencies in topics covered. What I find most interesting about this encyclopedia, though, is that it tends to "grow" on the reader; some of us felt downright giddy about this work after spending a week perusing it. I can highly recommend it to anyone who is interested in either physical chemistry or computational chemistry, regardless of whether they are a seasoned professional or a novice wanting to gain entry into the world of theory, informatics, and molecular simulation.

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